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PREDICTING POLYMER PROPERTIES
BY COMPUTATIONAL METHODS
I. POLYVINYL CHLORIDE AND
ITS HOMOLOGS

P.N. Krishnan
R.E. Morris

COPPIN STATE COLLEGE
Baltimore, MD 21216

G.R. Famini
A. Birenzvige

RESEARCH DIRECTORATE

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Krishnan, P.N., and Morris, R.E. (Coppin State College);
Famini, G.R., and Birenzvige, A. (CRDEC)

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A semiempirical quantum mechanical approach [semiempirical minimum neglect differential overlap (MNDO) Hamiltonian] has been applied to predict the heat of formation, dipole moment, polarizability, and solubility of polyvinyl chloride (PVC) and several of its homologs. Some of the physical properties of long chain polymers can be estimated from the calculations, using the dimer as a model. To the best of our knowledge, this study is the first attempt to predict polymer properties from relatively small molecule properties.

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PREFACE

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PREDICTING POLYMER PROPERTIES
BY COMPUTATIONAL METHODS
I. POLYVINYL CHLORIDE AND ITS HOMOLOGS

1.   INTRODUCTION

        Microencapsulation is a process of encasing (encapsulating) a chemical
by a high molecular weight polymeric material. The encapsulated chemical is
called "fill material," whereas the encapsulating polymer is called "shell."[1]
Microencapsulation is used in many diverse industries [e.g., paper (carbonless
carbon paper), pharmaceutical (time released medication and targeted drug
application), agricultural (time released herbicides and pesticides), and
perfume (scratch and sniff)]. The properties and applications of the
microcapsule greatly depend on the characteristics of its shell. The
possibilities of using microencapsulation on the chemical/biological battlefield
has been raised.

        Presently, development of new applications for microencapsulation
depends either on personal experience or a "hit and miss" approach to determine
the nature of the shell material. This report describes the initial results of
a study attempting to develop a systematic methodology using computational
chemistry for screening polymeric shell materials for their desired properties.

        Recent development of affordable high speed computer hardware and
"user friendly" software makes it possible to apply computational methods to
predict physical and chemical properties that are timely and expensive to
obtain experimentally in the laboratory. Also, the increased environmental
awareness and the proliferation of regulations for environmental protection
make the computational approach much more attractive. The application of one
computational method [Modified Neglect Differential Overlap (MNDO)] to predict
certain physical properties of polyvinyl chloride (PVC) and certain vinyl
chloride-ethylene copolymers is described in this report.

        The computational methods used in this work are described in Section 2.
The results and the discussion of the results are given in Section 3. The
report closes with a summary of the "experimental" work and recommendations for
future work.

2.   METHODS OF COMPUTATION

        Because of the limited computer resources existing, it is impractical
or even impossible to calculate the properties of the polymer. Thus, the
properties of shorter chains (monomer, dimer .... pentamer) were calculated in
an attempt to determine how the properties of the chain change with an
increasing number of monomer units and how many monomer units are required to
estimate the polymer properties.

        The molecules examined are large, making abinitio calculations
prohibitive. Therefore, semiempirical techniques employing MNDO Hamiltonian[2]
have been used to calculate the physical properties. The molecular geometry of
each molecule was optimized (see Appendix A) to give a minimum energy
conformation. Next, the MOPAC program[3] was used to calculate the heat of

formation, dipole moment, and polarization volume. The molecular volumes were calculated from the optimized geometries, using the Hopfinger algorithm[4] that is incorporated in the Molecular Modeling Analysis Display System (MMADS).[5,6,*] The molecular electrostatic potential (MEP) and the molecular lipophilic potential (MLP) for each molecule were calculated on a VdW Surface of the molecule.[2] The MEP was computed using the appropriate columbic potential ($V(r)$) in equation 1

$$V(\vec{r}) = \sum_{i} \frac{q_i}{\vec{r}_i} \tag{1}$$

where q_i is the formal charge of atom i and r_i is the distance from atom i to the point being examined. The MLP was determined using an analogous procedure. However, instead of q_i, the Hansch-Leo octanol/water partition coefficient values (l_i) for specific fragments were used

$$L_p(\vec{r}) = \sum_{l} \frac{l_i}{\vec{r}_i} \tag{2}$$

where $L_p(r)$ is the lipophilic potential, and l_i is the octanol/water coefficient for atom i (from Hansch-Leo fragment table), and r_i is the same as in equation 1.[7] Both MEP and MLP were examined on a Tektronic 4105 Color-graphic terminal. The calculations were performed on either a micro Vax II at U.S. Army Chemical Research, Development and Engineering Center (CRDEC) or on the Coppin State College (Baltimore, MD) Vax 780, both running under the VMS operating system.

3.   RESULTS AND DISCUSSIONS

3.1   Molecules Investigated.

        As stated before, the purpose of the current investigation is to determine if semiempirical methods could be used to estimate the different chemical and physical properties of polymeric materials used as shell material in microencapsulation. Because polymers are large molecules containing hundreds of atoms, it is desirable to predict these quantities from calculations performed on smaller molecules. Hence, calculations were performed on different oligomers (e.g., monomer, dimer, trimer, etc.) of vinyl chloride. In addition, compounds representing different degrees of chlorine substitution in the polymeric chain were chosen to examine how these substitutions affect the different chemical and physical properties. Table 1 lists the molecules investigated in the present study.

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* Molecular volume is that taken up by a molecule in space by adding the van de Waal's contribution for each atom and subtracting out the overlap volume.

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Table 1. Molecules Investigated

No.	Molecule Name	Molecular Structure
1.	Vinyl Chloride (Monomer)	$CH_2==CHCl$
2.	Ethyl Chloride	CH_3CH_2Cl
3.	1,3-Chloro Butane (Dimer)	$CH_2ClCH_2CHClCH_3$
4.	1,3,5-Chloro Hexane (Trimer)	$CH_2ClCH_2CHClCH_2CHClCH_3$
5.	1,3,5,7-Chloro Octane (Tetramer)	$CH_2ClCH_2CHClCH_2CHClCH_2CHClCH_3$
6.	1,3,5,7,9-Chloro Decane (Pentamer)	$CH_2ClCH_2CHClCH_2CHClCH_2CHClCH_2CHClCH_3$
7.	1-Chloro Butane	$CH_2ClCH_2CH_2CH_3$
8.	2-Chloro Butane	$CH_3CH_2CHClCH_3$
9.	1-Chloro Hexane	$CH_2ClCH_2CH_2CH_2CH_2CH_3$
10.	2-Chloro Hexane	$CH_3CHClCH_2CH_2CH_2CH_3$
11.	3-Chloro Hexane	$CH_3CH_2CHClCH_2CH_2CH_3$
12.	1,3-Chloro Hexane	$CH_2ClCH_2CHClCH_2CH_2CH_3$
13.	1,5-Chloro Hexane	$CH_2ClCH_2CH_2CH_2CHClCH_3$
14.	1,7-Chloro Octane	$CH_2ClCH_2CH_2CH_2CH_2CH_2CHClCH_3$
15.	1,5,7 Chloro Octane	$CH_2ClCH_2CH_2CH_2CHClCH_2CHClCH_3$
16.	1,7-Chloro Decane	$CH_2ClCH_2CH_2CH_2CH_2CH_2CHClCH_2CH_2CH_3$
17.	1,9-Chloro Decane	$CH_2ClCH_2CH_2CH_2CH_2CH_2CH_2CHClCH_3$
18.	1,5,9-Chloro Decane	$CH_2ClCH_2CH_2CH_2CHClCH_2CH_2CH_2CHClCH_3$

3.2   Geometry Optimization.

The properties of a compound depend strongly on its geometry. Thus, the first task was to determine the geometric structure of the molecule, which was determined by the method of energy minimization utilizing approximate methods (CRUDE). The calculated geometry was inspected visually to insure linearity of the hydrocarbon chain. If the chain was not linear, the dihedral angles between the four carbon atoms were adjusted to 180°. Then, MOPAC was used to obtain the final optimized geometry. These corrected geometries were used to calculate the various properties described below. The optimized geometries are presented in Appendix A.

3.3   Heat of Formation.

The calculated and experimental values of heat of formation for the molecules studied are compared in Table 2. As can be seen, the agreement between calculated and experimental values is quite good. For oligomers of vinyl chloride, Sinke and Stull predicted that the heat of formation will decrease by 22.6 Kcal/mol/monomer unit added even though they did not present any data to support this claim. However, our calculations show that the additional heat of formation for each additional monomer unit is about half that value (when ethyl chloride is taken as a monomer). Furthermore, it appears that this incremental increase is leveling off to around 13.5 Kcal/mole for each monomer addition after two units (see the figure).

3.4   Dipole Moment.

The distribution of charge in a molecular system has great significance for its reactivity and is a function of its structure. The dipole moment is the principal experimental quantity related to the charge distribution in the molecule. The calculated and experimental values of dipole moment for the molecules studied are compared in Table 3. Only a few experimental values were found in the literature. As can be seen, these values agree to within 0.5 Debye with the calculated values. Because the calculated dipole moment is a function of the postulated geometry of the molecule, this agreement supports the validity of the optimized geometries.

3.5   Polarizability.

Polarizability is an expression of the ability of an external electric field to induce a dipole moment (i.e. a charge separation in the molecule). As with dipole moment, very few experimental values are reported in the literature. For those molecules for which experimental values could be found, the agreement with the calculated values is reasonably good, as can be seen in Table 4.

Because it is an expression of the induced dipole moment, polarizability can be expected to depend on the size of the molecule. However, for oligomer composed of increasing numbers of the same or similiar building blocks, we can expect that the polarizability per unit volume will be similiar. The last column in Table 4, the polarizability index, is an expression of "unit polarizability" and is calculated by dividing the calculated polarization

Table 2. Molecular Heat of Formation

No.	Molecule Name	Calculated ΔH_f (Kcal/mol)	Experimental ΔH_f (Kcal/mol)
1.	Vinyl Chloride (Monomer)	4.94	8.07 ± 0.33[10-12]
2.	Ethyl Chloride	-28.8	-26.1 ± 0.51[10-12]
3.	1,3-Chloro Butane (Dimer)	-44.02	
4.	1,3,5-Chloro Hexane (Trimer)	-58.15	
5.	1,3,5,7-Chloro Octane (Tetramer)	-71.92	
6.	1,3,5,7,9-Chloro Decane (Pentamer)	-85.60	
7.	1-Chloro Butane	-38.49	-36.94 ± 0.281[10-12]
8.	2-Chloro Butane	-38.90	-38.53 ± 2.0[10-12]
9.	1-Chloro Hexane	-47.44	-48.59 ± 0.36[10-12]
10.	2-Chloro Hexane	-45.17	-48.80 ± 1.7[10-12]
11.	3-Chloro Hexane	-44.18	
12.	1,3-Chloro Hexane	-52.42	
13.	1,5-Chloro Hexane	-53.83	
14.	1,7-Chloro Octane	-63.35	
15.	1,5,7-Chloro Octane	-68.04	
16.	1,7-Chloro Decane	-71.55	
17.	1,9-Chloro Decane	-72.78	
18.	1,5,9-Chloro Decane	-77.56	
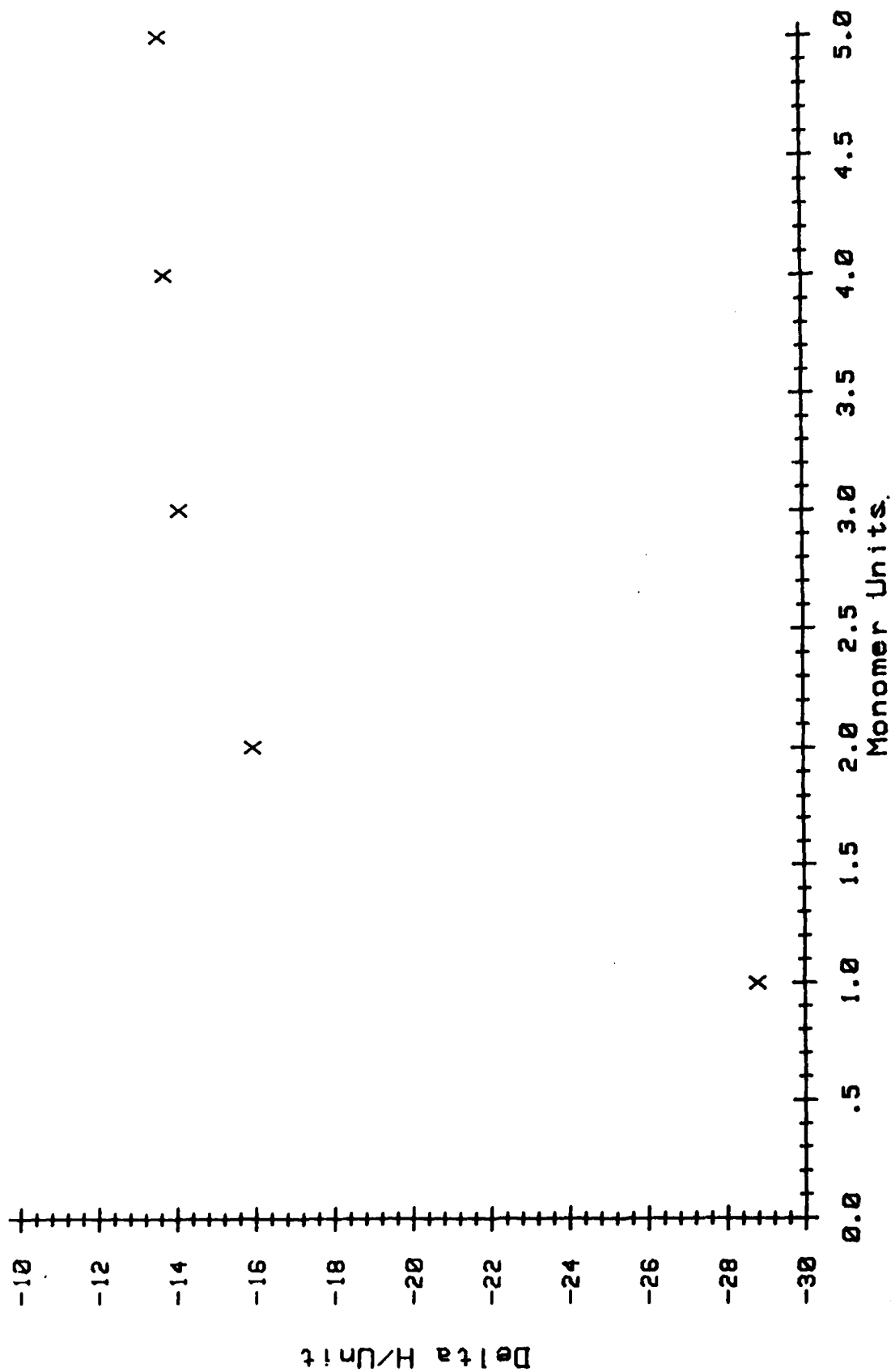
Figure. Change in H_f/Monomer Units

Monomer Units.

Delta H/Unit

Table 3. Dipole Moment

No.	Molecule Name	Calculated Dipole Moment (Debye)	Experimental Dipole Moment (Debye)
1.	Vinyl Chloride (Monomer)	1.70	1.45[9]
2.	Ethyl Chloride	1.55	2.05[10]
3.	1,3-Chloro Butane (Dimer)	2.11	
4.	1,3,5-Chloro Hexane (Trimer)	2.04	
5.	1,3,5,7-Chloro Octane (Tetramer)	2.86	
6.	1,3,5,7,9-Chloro Decane (Pentamer)	3.39	
7.	1-Chloro Butane	2.16	2.05[10]
8.	2-Chloro Butane	2.12	2.04[10]
9.	1-Chloro Hexane	2.05	
10.	2-Chloro Hexane	2.09	
11.	3-Chloro Hexane	2.05	
12.	1,3-Chloro Hexane	2.23	
13.	1,5-Chloro Hexane	2.18	
14.	1,7-Chloro Octane	2.28	
15.	1,5,7-Chloro Octane	2.06	
16.	1,7-Chloro Decane	2.49	
17.	1,9-Chloro Decane	2.33	
18.	1,5,9-Chloro Decane	2.08	

Table 4. Polarization Volume, Molecular Volume, and Polarizability Index

No.	Molecule Name	Calculated Polarization Volume	Experimental Polarization Volume[10]	Molecular Volume	Polarizability Index
1.	Vinyl Chloride (Monomer)	5.84	6.41	55.4	0.105
2.	Ethyl Chloride	6.30	7.27	62.3	0.053
3.	1,3-Chloro Butane (Dimer)	12.00		113.7	0.106
4.	1,3,5-Chloro Hexane (Trimer)	17.69		164.5	0.108
5.	1,3,5,7-Chloro Octane (Tetramer)	23.33		215.4	0.108
6.	1,3,5,7,9-Chloro Decane (Pentamer)	28.98		266.3	0.109
7.	1-Chloro Butane	10.01	11.3	98.3	0.102
8.	2-Chloro Butane	10.06	12.4	98.3	0.102
9.	1-Chloro Hexane	13.78		131.7	0.105
10.	2-Chloro Hexane	13.82		133.8	0.103
11.	3-Chloro Hexane	13.80		133.7	0.103
12.	1,3-Chloro Hexane	15.77		149.1	0.106
13.	1,5-Chloro Hexane	15.79		149.1	0.106
14.	1,7-Chloro Octane	19.58		184.9	0.106
15.	1,5,7-Chloro Octane	21.47		200.0	0.107
16.	1,7-Chloro Decane	23.35		215.0	0.109
17.	1,9-Chloro Decane	23.38		220.1	0.106
18.	1,5,9-Chloro Decane	25.26		235.6	0.107

volume (Column 3) by the calculated molecular volume (Column 5). As can be seen, the polarizability indices of all the molecules studied, except ethyl chloride, fall within 3% of the average value of 0.016.

3.6   Solubility.

The distribution of electrons around the molecule determine the reactivity of the molecule. In general, a homogenous distribution indicates low reactivity, but a concentration of charge at certain regions will indicate high reactivity. Similarly, a homogenous charge distribution will indicate low solubility in a polar solvent such as water.

By plotting the electrostatic and lipophilic potential around the molecule, we can qualitatively assess the chemical reactivity and polar solubility of the compound.[14-19] The MEP and MLP maps for the molecules investigated indicate that they all have very low solubility in water, which is confirmed in Table 5. As expected, the solubility in water diminishes with an increasing number of carbon atoms in the chain. Similarly, the MEP maps indicate that the molecules investigated have very low reactivity, which is also expected.

4.   CONCLUSIONS

The results of this semiempirical study indicate that oligomers as small as the dimer can be used as a model to reasonably predict at least some of the physical properties of PVC. It appears that vinyl chloride can not be used as a model for PVC due to the large deviation of the heat of formation. Ethyl chloride is eliminated as a potential model because of the discrepancy in the dipole moment and polarizability index. The MEP and MLP maps confirm the similarity between the dimer and the larger chain PVC molecules. These maps also confirm the dissimilarities between the vinyl chloride, ethyl chloride, and longer chain PVC molecules. This is the first known attempt to predict the behavior of polymers based on calculations of the properties of shorter chain molecules. The vinyl chloride-ethylene copolymers investigated here show similar properties to the PVC.

5.   RECOMMENDATIONS

This study shows that computational chemistry can be used to estimate physical and chemical properties of polymeric compounds. The semi-empirical computer model used in this effort is the MNDO. However, other computer models, which are available, should be investigated. Determining which model is best suited to predict each property is the subject of an ongoing investigation and will be reported upon at a later date. We recommend that a methodology to estimate the solubility of polymeric materials in different media be developed with similar calculations performed on other polymeric materials. To investigate the predictability of spectral excitation frequencies for polymeric materials, these calculations should be extended to the abinitio level.

Table 5. Solubility

No.	Molecule Name	Experimental Solubility (% W/W)
1.	Vinyl Chloride (Monomer)	0.27[11]
2.	Ethyl Chloride	0.447[11]
3.	1,3-Chloro Butane (Dimer)	
4.	1,3,5-Chloro Hexane (Trimer)	
5.	1,3,5,7-Chloro Octane (Tetramer)	
6.	1,3,5,7,9-Chloro Decane (Pentamer)	
7.	1-Chloro Butane	0.11[11]
8.	2-Chloro Butane	0.10[11]
9.	1-Chloro Hexane	0.008[13]
10.	2-Chloro Hexane	
11.	3-Chloro Hexane	
12.	1,3-Chloro Hexane	
13.	1,5-Chloro Hexane	
14.	1,7-Chloro Octane	
15.	1,5,7-Chloro Octane	
16.	1,7-Chloro Decane	
17.	1,9-Chloro Decane	
18.	1,5,9-Chloro Decane	

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OPTIMIZED GEOMETRIES OF VARIOUS MOLECULES
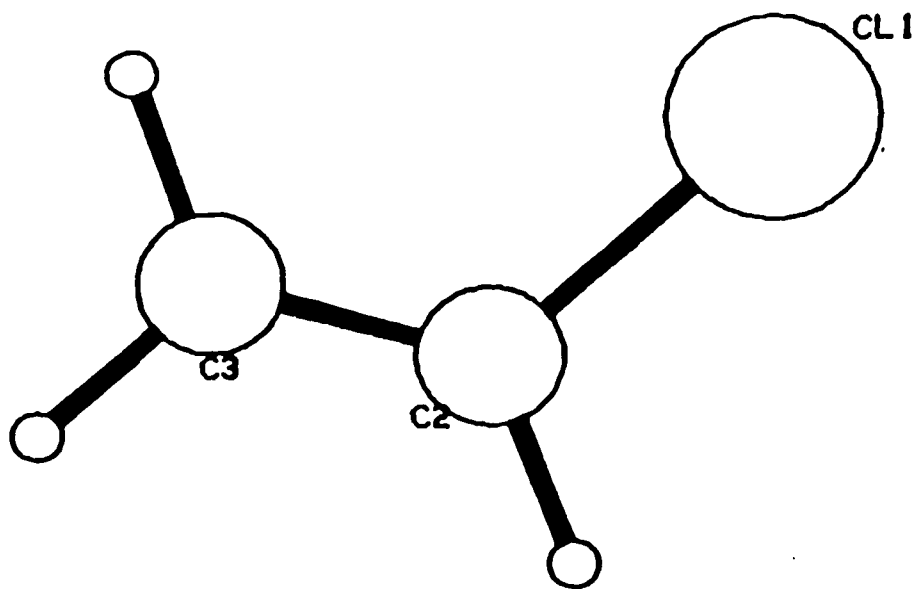
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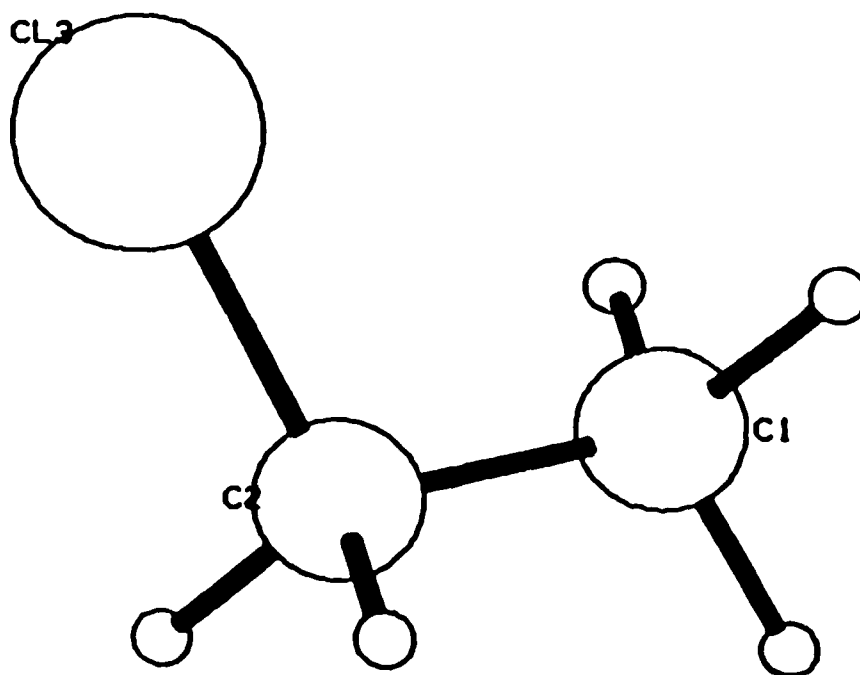
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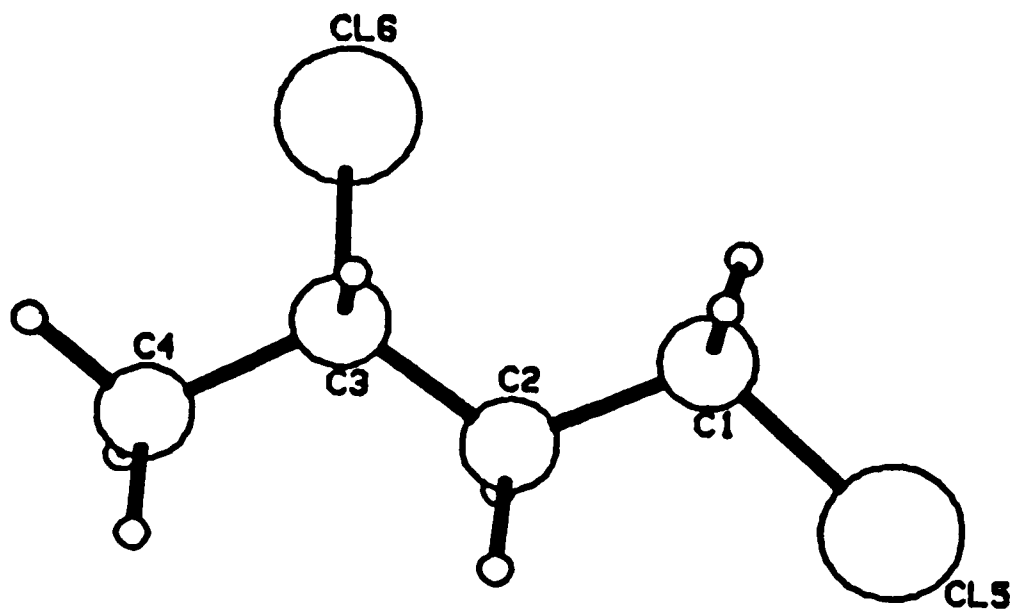
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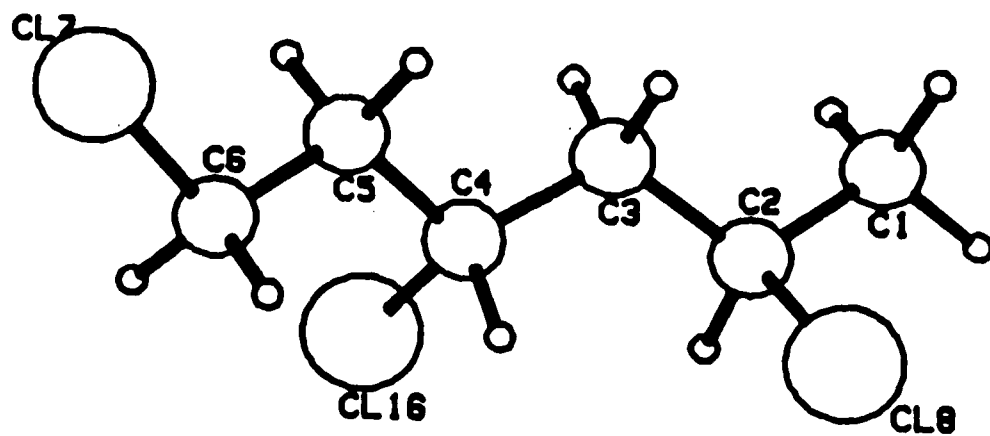
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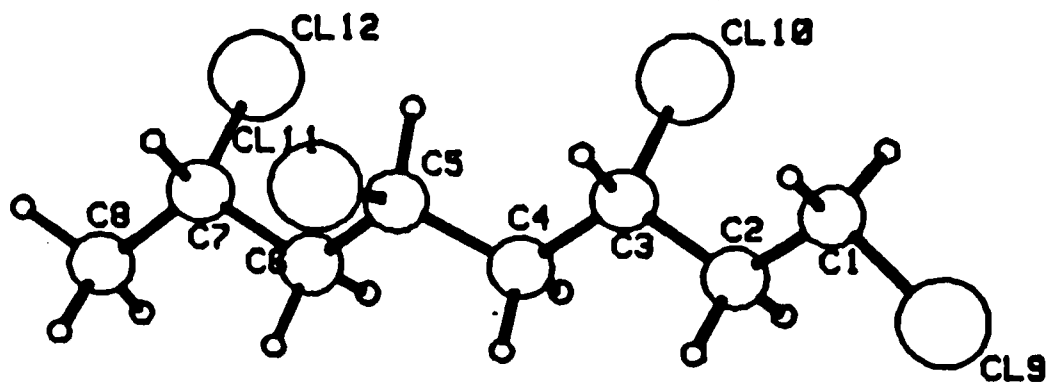
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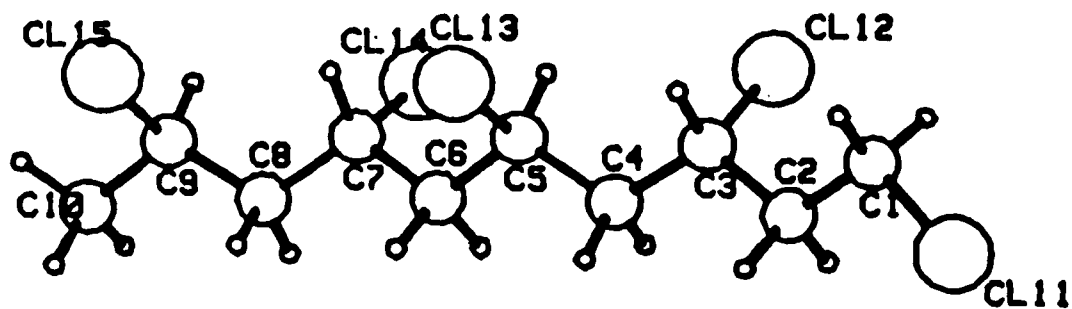
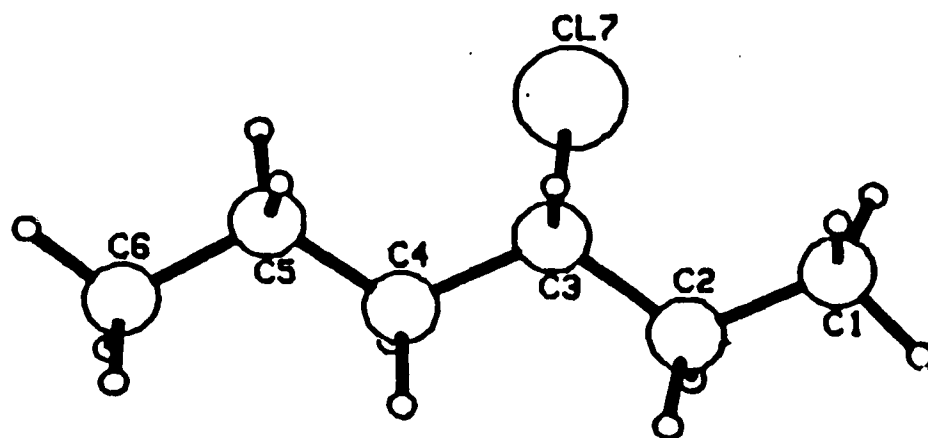1, 3, 5, 7, 9 – CHLORODECANE (Pentamer)
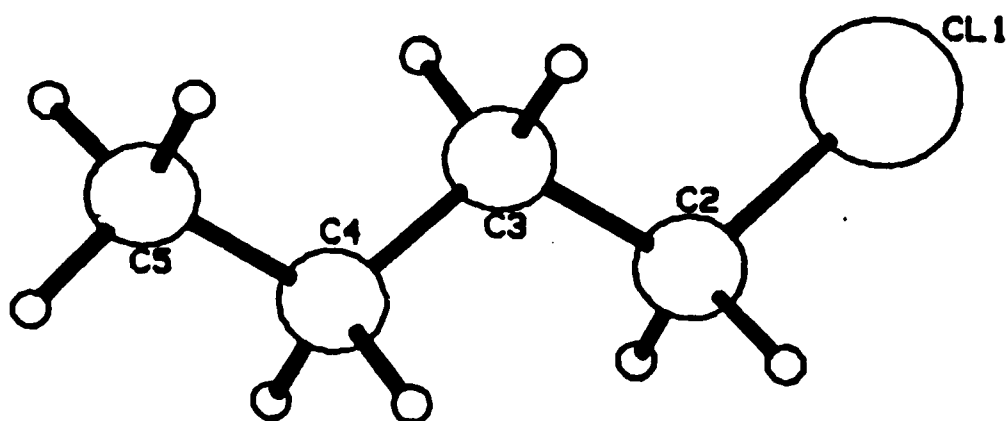
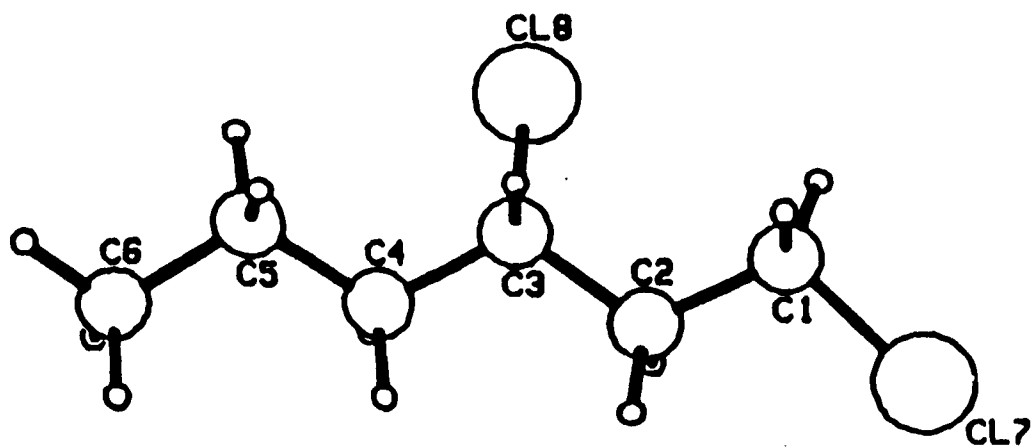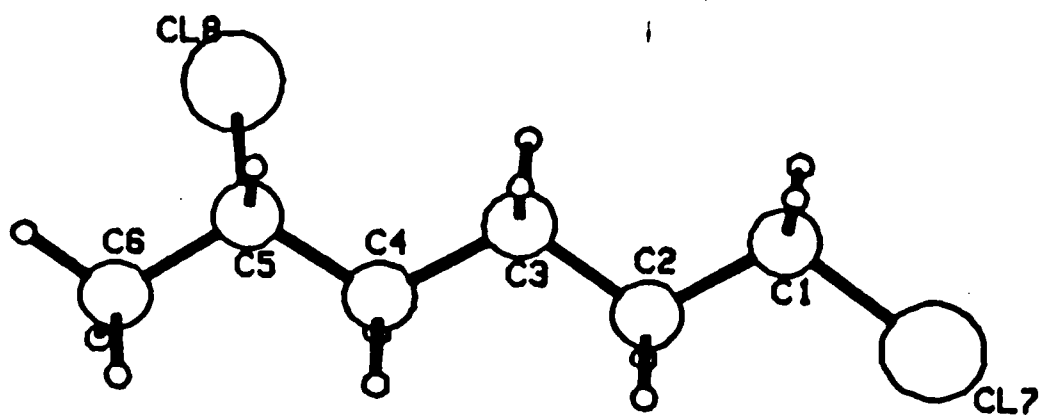1- CHLOROBUTANE
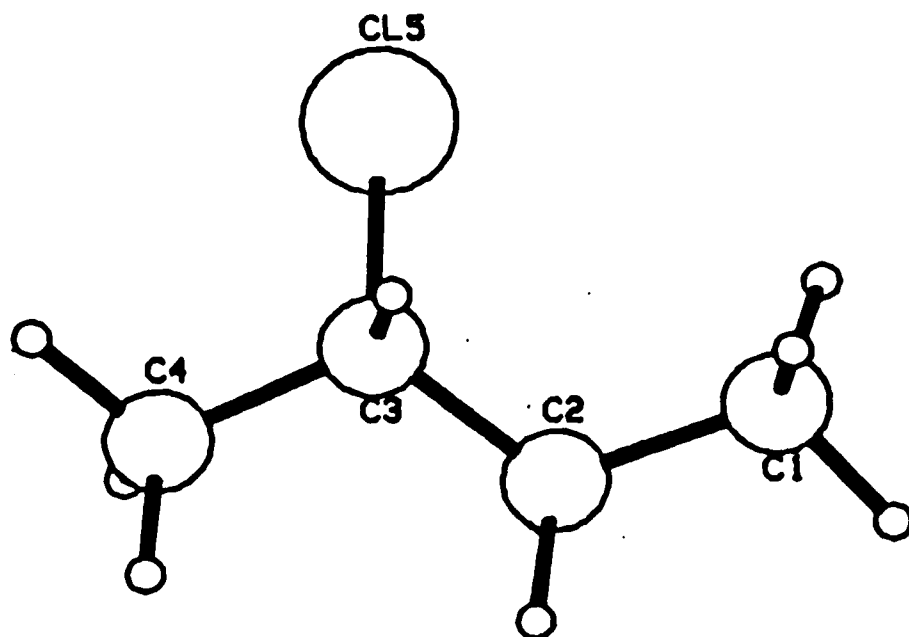
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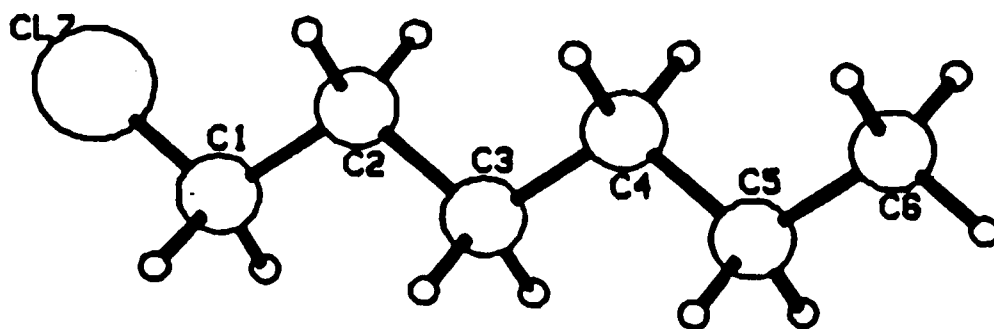
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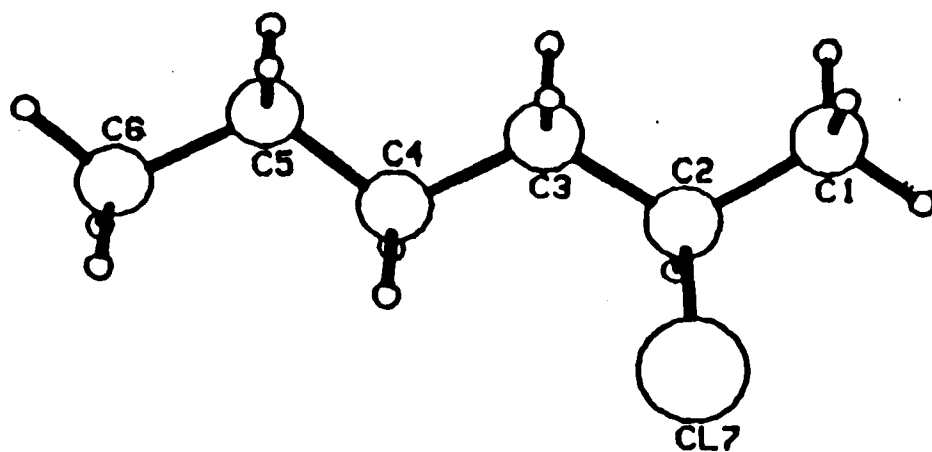
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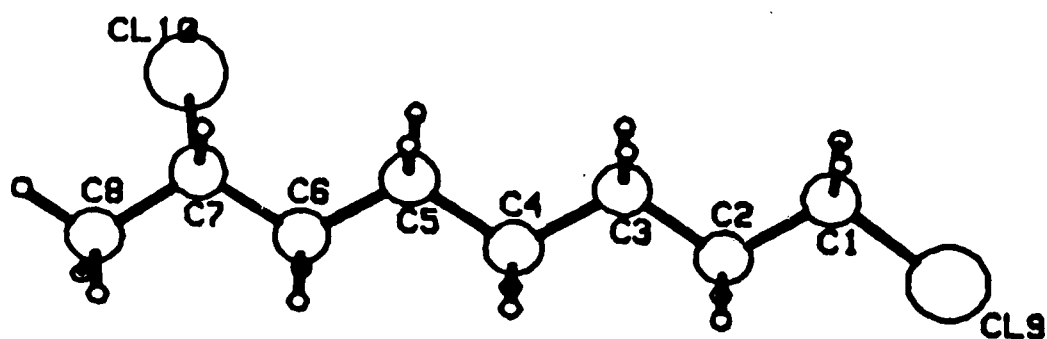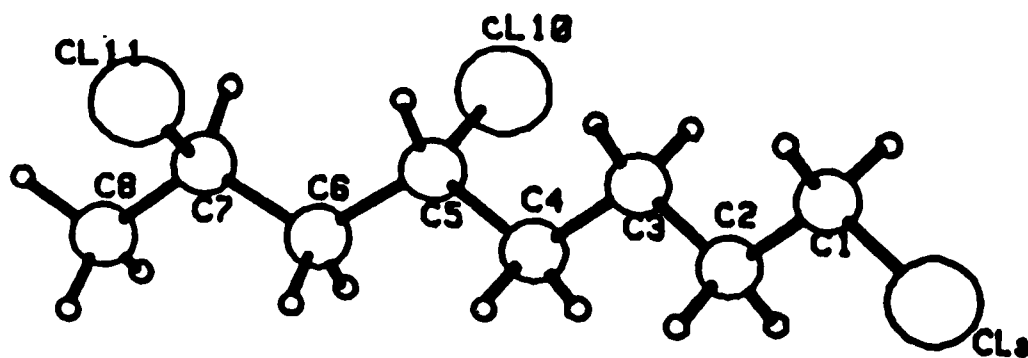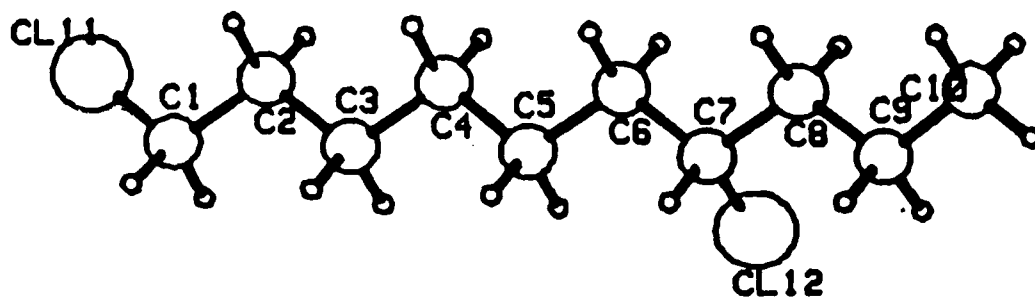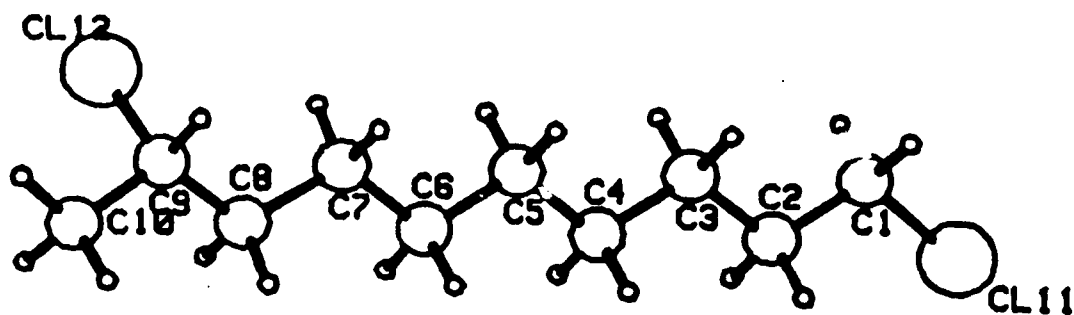

3 - CHLOROHEXANE

1, 3 - CHLOROHEXANE

1, 5 – CHLOROHEXANE
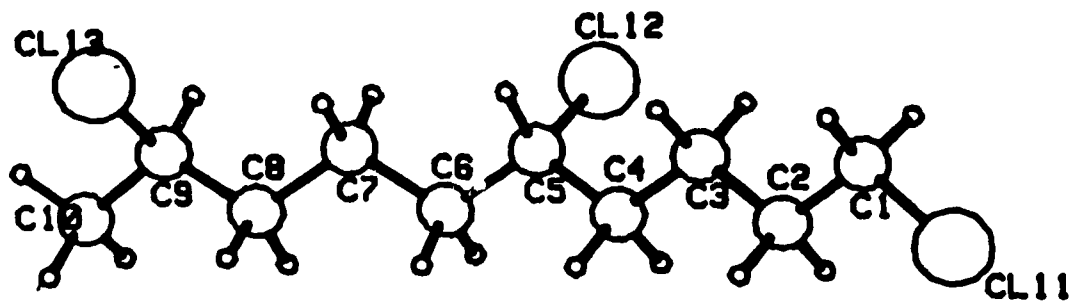

1, 7 – CHLOROHEXANE

1, 5, 7 – CHLORO OCTANE

1, 7 – CHLORO DECANE

1, 9 – CHLORO DECANE

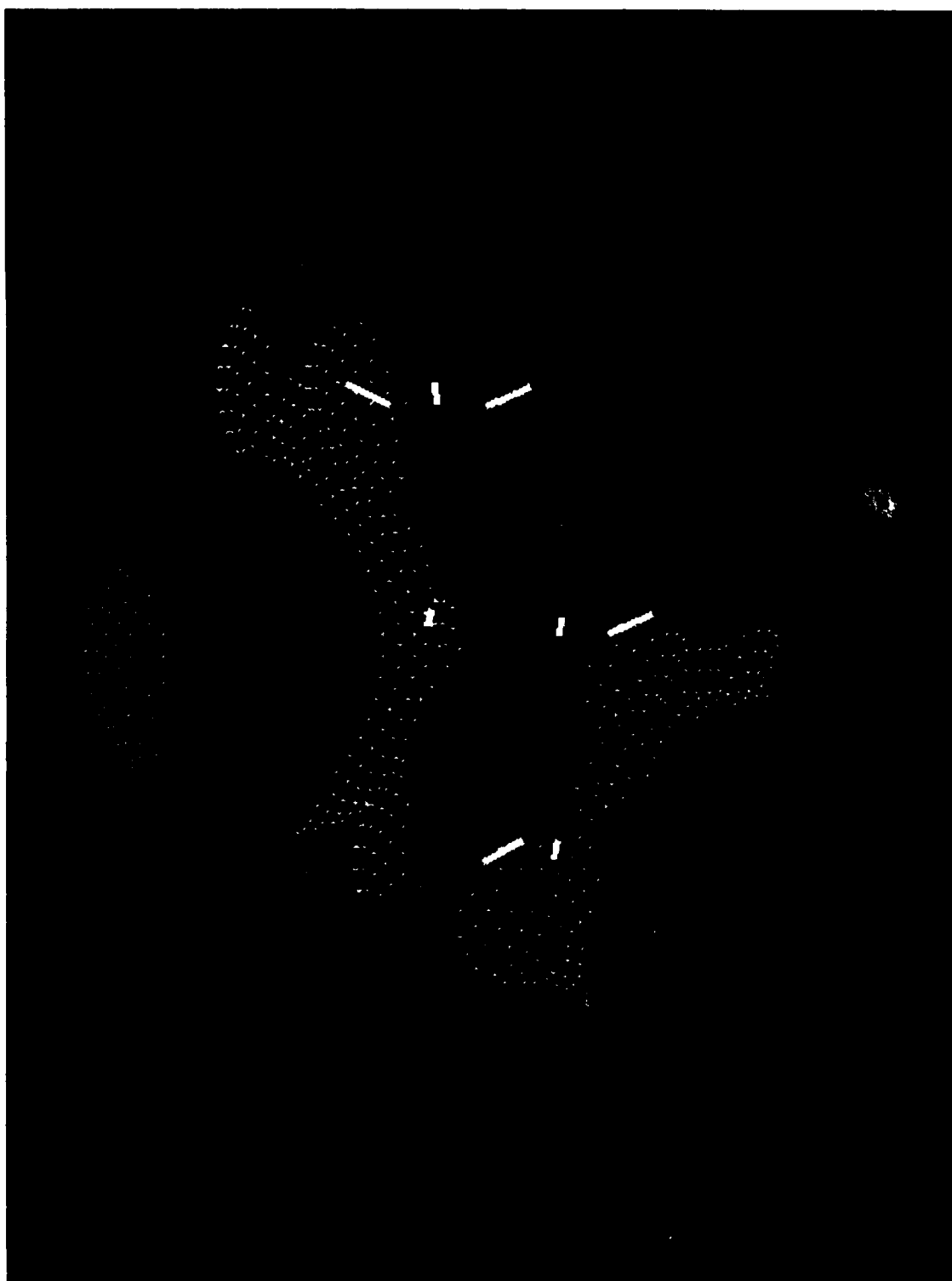1, 5, 9 – CHLORO DECANE

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APPENDIX B

MOLECULAR ELECTROSTATIC POTENTIAL AND
MOLECULAR LIPOPHILIC POTENTIAL MAPS

The potential at a point on the molecular surface is represented by color coding; red is used to represent the most negative potential and blue, the most positive. The other colors of the spectrum represent values between the two extremes. Therefore, through visual inspection of the molecular electrostatic potential maps, one can equate significant charge separations with large polarization (reactivity).

Similarly, the molecular lipophilic potential maps represent insoluble portions of the molecule with violet and soluble portions with red. Again, visual inspection is used to determine the solubility of the molecule.

MEP: 1,3-Chloro Butane (Dimer)

MEP: 1,3,5,7,9-Chloro Decane (Pentamer)

MLP: 1,3-Chloro Butane (Dimer)

MLP: 1,3,5,7,9-Chloro Decane (Pentamer)